## OAK RIDGE NATIONAL LABORATORY MANAGED BY UT-BATTELLE, LLC POST OFFICE BOX 2008, OAK RIDGE, TENNESSEE 37831-6170

# ORNL FOREIGN TRIP REPORT TA 421 817

**DATE:** June 1, 2018

**SUBJECT:** Report of Foreign Travel to Paris and Fontenay aux Roses, France – Vladimir Sobes,

Reactor and Nuclear Systems Division

**TO:** Angela Chambers, Nuclear Criticality Safety Program Manager, National Nuclear

Security Administration / NA-511/GTN, Pantex Plant, PO Box 30020, Amarillo, TX

79120-0020

FROM: Vladimir Sobes

**MEETING:** OECD/NEA Working Party on Nuclear Data Evaluation Cooperation (WPEC)

TITLE Meeting and NCSP Nuclear Data Collaboration with IRSN

**MEETING:** OECD Conference Center, Paris, France; Institute of Radiological protection and

**LOCATION** Nuclear Safety (IRSN), Fontenay Aux Roses, France

**MEETING:** 05/14/2018 - 06/01/2018

**DATES** 

**ATTENDEES:** Vladimir Sobes

ON BEHALF OF NCSP

MEETING:

**BENEFIT TO** 

NCSP

The benefit of this travel is that it supports the Mission and Vision of the Nuclear Criticality Safety Program in a number of ways. Foremost, this travel supports the Mission of the Nuclear Data technical program element through the coordination of nuclear data activities and fostering a strong collaborative effort among international resources via active participation in the OECD/NEA Working Party Evaluation Cooperation (WPEC) expert working groups. Furthermore, this travel supports the ORNL Nuclear Data Milestone, ORNL-ND1, as detailed in the NCSP Five Year Execution Plan. The main purpose of the trip is for nuclear data research collaboration between ORNL and IRSN in support of timely completion of the nuclear data evaluations listed in the Appendix B of the Five Year Execution Plan. Details of the WPEC 2018 Meeting and collaboration with IRSN are provided below.

**MEETING PURPOSE:** 

The purpose of the first week of this trip is for Dr. Sobes to lead the meeting of the WPEC Subgroup 44 on the Investigation of Covariance Data in General Purpose Nuclear Data Libraries during the OECD/NEA WPEC 2018 Meeting. Dr. Sobes has been selected as the coordinator of this international subgroup. In this faculty, Dr. Sobes supports the Mission of the Nuclear Data technical program element of the NCSP by facilitating coordination of nuclear data activities by fostering a strong collaborative effort among international resources in this highly technical area. Active participation in the OECD/NEA Working Party Evaluation Cooperation (WPEC) expert working groups is explicitly called out in the NCSP Mission and Vision document. The mandate of Subgroup 44 sets out to improve nuclear data covariance

evaluations in general purpose nuclear data libraries, such as the ENDF/B library used by practitioners of nuclear criticality safety in the US. Quality nuclear data covariance information is essential to establishing safety margins in criticality calculations. The benefit to the NCSP is the exchange information with international NCS community to improve NCSP nuclear data work and cultivate new collaborations to support future NCSP nuclear data tasks which is in accordance with the specific milestone ORNL-ND1 set out in the NCSP Five Year Execution Plan FY2018-2022.

At the WPEC 2018 Meeting Dr. Sobes had also organized and coordinated two additional joint meeting with other WPEC Subgroups. In particular, in the morning of Tuesday, May 15, Dr. Sobes lead a joint meeting between his Subgroup 44 and Subgroup 46 on Efficient and Effective Use of Integral Experiments for Nuclear Data Validation. The two groups have overlap in the topic of the uses of integral experiments for covariance evaluation which prompted an active and productive discussion during the session the highlights of which are provided in the full report below. Both groups greatly benefited from the organization of the joint meeting.

On Tuesday afternoon, May  $15^{th}$ , Dr. Sobes lead a joint meeting between three different subgroups of the WPEC. In particular Subgroup 44 on Covariance meet with the members of Subgroup 42 on Thermal Scattering Kernel  $S(\alpha,\beta)$ : Measurement, Evaluation and Application and well as the NEA Expert Group on the Recommended Definition of a General Nuclear Data Structure (GNDS). This was a very important joint meeting to discuss, for the first time as a broader nuclear data community, a path forward for covariance data for thermal scattering law libraries. The highlights of the discussions are provided below.

On Wednesday, May 16, Dr. Sobes actively contributed to the activities of the Joint Meeting of Subgroups 39 and 46 on the uses of integral data for nuclear data adjustment and in the meeting of the Expert Group on the Nuclear Data High Priority Request List. Lastly, on Thursday and Friday, May 17-18, Dr. Sobes participated in the WPEC committee meeting coordinating the activities of the different WPEC subgroups and nuclear data research around the world.

The purpose of the collaboration visit to IRSN is for Dr. Sobes (ORNL) to collaborate with Dr. Luiz Leal (IRSN) on several nuclear data evaluation tasks listed in the NCSP Five Year Execution Plan FY2018-2022. Dr. Sobes is the PI at ORNL for the resonance region evaluation of <sup>156</sup>Gd, <sup>158</sup>Gd, and <sup>160</sup>Gd as indicated in Appendix B of the NCSP Five Year Plan and implied under the Milestone ORNL-ND1. Dr. Leal has been working in parallel on the resonance evaluation of <sup>155</sup>Gd and <sup>157</sup>Gd at IRSN. One of the objectives of this visit is for the two researchers to come together and synchronize their work, such that each can benefit from further working with the latest resonance parameters for the other isotopes of Gadolinium. The technical significance of this synchronization is that in the resonance analysis, experimental data are measured using natural samples and the analysis impacted by the resonances of all five isotopes. Therefore, it is natural, that changes to one or several of the isotopes will have an impact on the resonance parameters of the other isotopes. Thus, periodic synchronization is essential.

Sobes (ORNL) and Leal (IRSN) are have began the re-evaluation of the isotopes of lead as indicated in Appendix B. During this visit a comprehensive review of the

current evaluations in ENDF/B-VIII.0 and JEFF3.3 was performed. The effort culminated in a summary to be submitted to the ANS Winter Meeting and Technology Expo.

As part of the visit, Sobes and Leal were able to coordinate a session for the Nuclear Criticality Safety Division of the American Nuclear Society which they jointly proposed to organize for the ANS Winter Meeting and Technology Expo. The session is entitled New Code Developments for Nuclear Criticality Safety Applications. This session is well aligned with the vision of the NCSP in the Analytic Methods Focus Area.

The collaboration visit to IRSN also resulted in numerous spontaneous discussion and ideas for further collaboration of mutual benefit to both ORNL/NCSP and IRSN. Some of these included discussions of the upcoming evaluations of Tantalum and Molybdenum. Dr. Leal contributed to a new approach to determine the resonance quantum angular momentum and parity for the <sup>56</sup>Fe that Dr. Sobes is proposing to develop through external funding (at no cost to NCSP). Discussion were held about Thermal Scattering Law Libraries and the upcoming visit of IRSN staff to the Spallation Neutron Source at ORNL. Further, a very beneficial discussion happened about cross-validating the processing of nuclear data in the Unresolved Resonance Region between AMPX (ORNL) and GAIA (IRSN). Both groups have seen similar problems. Lastly, a potential future collaboration was discussed on resonance parameter sensitivity calculations currently being implemented in the CE TSUNAMI-3D module of the SCALE code system under an ORNL Seed Money Grant (at no cost to NCSP).

SITES NEA Headquarters, Paris, France VISITED: IRSN, Fontenay aux Roses, France

**ABSTRACT:** 

The traveler made a trip to the Institute of Radiological protection and Nuclear Safety (IRSN) to work collaboratively with the IRSN nuclear data team on the cross section evaluations in the resolved resonance region for isotopes of interest to NCSP and IRSN. In particular, gadolinium and lead. The traveler also was responsible for leading the meeting of WPEC Subgroup 44 on the "Investigation of Covariance Data in General Purpose Nuclear Data Libraries" during the WPEC 2018 Meeting at the OECD Conference Center. The traveler organized and coordinated two other joint meetings between different WPEC subgroups to discuss the uses of integral data in covariance evaluations and to break group on establishing a thermal scattering law covariance data libarary.

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### REPORT OF FOREIGN TRAVEL

### Vladimir Sobes Fontenay aux Roses, France November 20, 2017 – December 1, 2017

### **PURPOSE OF TRAVEL**

The benefit of this travel is that it supports the Mission and Vision of the Nuclear Criticality Safety Program in a number of ways. Foremost, this travel supports the Mission of the Nuclear Data technical program element through the coordination of nuclear data activities and fostering a strong collaborative effort among international resources via active participation in the OECD/NEA Working Party Evaluation Cooperation (WPEC) expert working groups. Furthermore, this travel supports the ORNL Nuclear Data Milestone, ORNL-ND1, as detailed in the NCSP Five Year Execution Plan. The main purpose of the trip is for nuclear data research collaboration between ORNL and IRSN in support of timely completion of the nuclear data evaluations listed in the Appendix B of the Five Year Execution Plan.

The purpose of the first week of this trip is for Dr. Sobes to lead the meeting of the WPEC Subgroup 44 on the Investigation of Covariance Data in General Purpose Nuclear Data Libraries during the OECD/NEA WPEC 2018 Meeting. Dr. Sobes has been selected as the coordinator of this international subgroup. In this faculty, Dr. Sobes supports the Mission of the Nuclear Data technical program element of the NCSP by facilitating coordination of nuclear data activities by fostering a strong collaborative effort among international resources in this highly technical area. Active participation in the OECD/NEA Working Party Evaluation Cooperation (WPEC) expert working groups is explicitly called out in the NCSP Mission and Vision document. The mandate of Subgroup 44 sets out to improve nuclear data covariance evaluations in general purpose nuclear data libraries, such as the ENDF/B library used by practitioners of nuclear criticality safety in the US. Quality nuclear data covariance information is essential to establishing safety margins in criticality calculations. The benefit to the NCSP is the exchange information with international NCS community to improve NCSP nuclear data work and cultivate new collaborations to support future NCSP nuclear data tasks which is in accordance with the specific milestone ORNL-ND1 set out in the NCSP Five Year Execution Plan FY2018-2022.

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Three of the highlights from the Subgroup 44 meeting led by Dr. Sobes are summarized below. 1) The first steps were taken in coordinating the inclusion of cross correlations between incident neutron energies in the Prompt Fission Neutron Spectra in the ENDF/B-VIII.0 <sup>239</sup>Pu evaluation. Subgroup 44 will work towards identifying how to store and use such data. Further, the important question to the mission of the NCSP that Subgroup 44 will aim to answer is what is the required fidelity of such covariance data such as to preserve all of relevant physics with impact to the uncertainty on the calculation of criticality safety applications. 2) Over the following year, Subgroup 44 will work to define computational exercise to determine the sources of discrepancies between the covariance evaluations of different nuclear data libraries. This computational exercise will involve international collaboration to answer the question of the practitioners of why different nuclear data covariance libraries result in different levels of certainty on nuclear systems modeling. 3) A discussion of an attempt to establish a validation procedure for covariance data began in the Subgroup 44 meeting and continued in the next joint meeting between Subgroups 44 and 46. This is an important step towards understanding the quality of covariance data in the libraries.

At the WPEC 2018 Meeting Dr. Sobes had also organized and coordinated two additional joint meeting with other WPEC Subgroups. In particular, in the morning of Tuesday, May 15, Dr. Sobes lead a joint meeting between his Subgroup 44 and Subgroup 46 on Efficient and Effective Use of Integral Experiments for Nuclear Data Validation. The two groups have overlap in the topic of the uses of integral experiments for covariance evaluation which prompted an active and productive discussion during the session. Both groups greatly benefited from the organization of the joint meeting.

The first deliverable to the WPEC of Subgroup 44 will be a high priority covariance evaluation list that will mirror and be coordinated with the High Priority Request List maintained by the NEA. This list can further be fed into the Nuclear Data Advisory Board of the NCSP as a guidance document coming from the international nuclear data community. The initial compilation of the entries of such a list was one of the major goals of the joint meeting between Subgroup 44 and Subgroup 46 based on the feedback from integral calculations. The agreed-upon process will be that Dr. Sobes compiles the list and circulates it through the international nuclear data community throughout the following year, established documentation of covariance discrepancies and needs.

On Tuesday afternoon, May  $15^{th}$ , Dr. Sobes lead a joint meeting between three different subgroups of the WPEC. In particular Subgroup 44 on Covariance meet with the members of Subgroup 42 on Thermal Scattering Kernel  $S(\alpha,\beta)$ : Measurement, Evaluation and Application and well as the NEA Expert Group on the Recommended Definition of a General Nuclear Data Structure (GNDS). This was a very important joint meeting to discuss, for the first time as a broader nuclear data community, a path forward for covariance data for thermal scattering law libraries.

In a 3+ hour active discussion many issues with developing, distributing and using covariance data for thermal scattering laws we brought up and some were resolved. Most importantly, the in joint meeting of the three subgroups, a clear path forward was established. Several of the research groups producing thermal scattering law libraries he taken an action to produce thermal scattering law covariance data and distribute to the participants of the meeting. From there the path forward forks in two directions. First, the distributed covariance files will be used as the seed for the generation of "random files" allowing for a first estimate of the amount of uncertainty coming from uncertainty in thermal scattering libraries. The second path will be for research groups developing processing codes to begin to develop capabilities to process the delivered thermal scattering law covariance data. Once processed the covariance data will be propagated to applications and compared to the results obtained from the use of random files.

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Expert Group on the Nuclear Data High Priority Request List. Lastly, on Thursday and Friday, May 17-18, Dr. Sobes participated in the WPEC committee meeting coordinating the activities of the different WPEC subgroups and nuclear data research around the world.

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As one quantitative example of the collaboration visit was the Sobes and Leal by joint efforts, managed to reduce the chi-squared statistical metric of the fit of experimental capture data from RPI from a value of 5.2 to below 4.5. Further, progress was made in the unresolved resonance region of <sup>156</sup>Gd and <sup>158</sup>Gd. The SAMINT code was initially developed under NCSP succession planning funding. During a previous collaboration visit to IRSN, Sobes and Leal extended the capabilities the SAMINT auxiliary code to include parameters of the unresolved resonance region. This capability can further be used to improve the unresolved resonance region evaluations of the isotopes of gadolinium.

Sobes (ORNL) and Leal (IRSN) are have began the re-evaluation of the isotopes of lead as indicated in Appendix B. During this visit a comprehensive review of the current evaluations in ENDF/B-VIII.0 and JEFF3.3 was performed. The effort culminated in a summary to be submitted to the ANS Winter Meeting and Technology Expo.

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Overall, Dr. Sobes' foreign travel to IRSN was successful and essential to enable ORNL to make progress on the planned NCSP nuclear data evaluation tasks (ORNL ND1) as defined in the NCSP Five-Year Plan Execution Plan FY2018-2022. The complete resonance region evaluations of the isotopes of <sup>155</sup>Gd, <sup>156</sup>Gd,

<sup>157</sup>Gd, <sup>158</sup>Gd and <sup>160</sup>Gd are currently estimated to be delivered at the end of FY2019 with a preliminary version of the new resonance evaluations being available in Q4 of FY2018.

### **Persons Contacted at IRSN**

Luiz Leal, Host Raphaelle Ichou Stephan Ivo Eric Dumonteil Vaibhav Jiswal Clément Jeannesson

**Itinerary** 

05/12/18 - 05/13/18 Travel from Knoxville, TN to Paris, France 05/14/18 - 05/18/18 WPEC 2018 Meeting. Conference agenda:

https://www.oecd-nea.org/science/wpec/meeting2018/

05/21/18 – 06/01/18 IRSN, Fontenay aux Roses, France (detailed agenda follows)

06/02/18 – 06/08/18 Personal travel (no cost to NCSP) 06/09/18 Return Paris, France to Knoxville, TN

IRSN, Fontenay aux Roses, France (detailed agenda)

05/21/18 - 05/23/18 Evaluation work on the isotopes of gadolinium.

Fitting of differential experimental data.

Review of literature for ENDF/B-VIII.0 and JEFF3.3 lead evaluations. Compilation of historical measurements of key evaluation parameters.

05/24/18 – 05/25/18 Review of EXFOR data base for differential cross section measurements for lead.

Calculation of the quantum angular momentum and parity for the isotopes of

lead.

Review of resonance parameter statistics for the existing evaluations.

Discussion of the URR evaluation for gadolinium.

Organization of the 2018 ANS Winter Meeting and Technology Expo Nuclear Criticality Safety Division session on New Code Developments for Nuclear

Criticality Safety Applications.

05/28/18 – 05/29/18 Synchronization of evaluated resonance parameters between <sup>156</sup>Gd, <sup>158</sup>Gd, and

<sup>160</sup>Gd (ORNL) and <sup>155</sup>Gd and <sup>157</sup>Gd (IRSN).

Review of performance improvements and differences.

Discussion of ongoing nuclear data evaluation efforts at ORNL and IRSN

including Gd, Pb, Ta, Mo, <sup>233</sup>U and V.

Discussion of a new method for the autonomous identification of the total

angular momentum and parity in the resonance region for <sup>56</sup>Fe.

05/30/18 – 05/31/18 Discussion of cross-validation of AMXP (ORNL) and GAIA (IRSN) processing

codes in the unresolved resonance region.

Discussion of future collaboration on resonance parameter sensitivity

calculations.

Drafting of the ANS summary highlighting the comprehensive study on the

evaluations of lead in ENDF/B-VIII.0 and JEFF3.3

06/01/18 Final discussions and future collaborations.

Review and editing of the ANS summary on lead.

Writing of the Foreign Travel Report.

### **DISTRIBUTION**

- 1. Doug G. Bowen (<u>bowendg@ornl.gov</u>)
- 2. Angela Chambers (<u>angela.chambers@nnsa.doe.gov</u>)
- 3. Lori Scott (Lorisc0tt@aol.com)

## OAK RIDGE NATIONAL LABORATORY MANAGED BY UT-BATTELLE, LLC POST OFFICE BOX 2008, OAK RIDGE, TENNESSEE 37831-6170

# ORNL FOREIGN TRIP REPORT TA

DATE: SUBJECT:

**TO:** Angela Chambers, Nuclear Criticality Safety Program Manager, National Nuclear

Security Administration / NA-511/GTN, Pantex Plant, PO Box 30020, Amarillo, TX

79120-0020

**FROM:** Dorothea Wiarda

**MEETING:** 30th WPEC Meetings

TITLE

**MEETING:** OECD Conference Center, 2, rue André Pascal – 75016 Paris

LOCATION

**MEETING:** 05/14/18 - 05/18/18

DATES

**ATTENDEES:** Dorothea Wiarda

ON BEHALF OF NCSP MEETING: BENEFIT TO

NCSP

**MEETING** Participate in the sub-group meetings for the OECD/NEA Working Party Evaluation Cooperation (WPEC), specifically: SG-43, EG-GNDS, SG-44, and

SG-45. EG-GNDS was established for the long-time governance of the ENDF/GNDS format. The SG-43 was established to provide and API and physics checks for the new ENDF format. The data processing code AMPX, used to generate cross section libraries for SCALE and the analysis code SAMMY, both of which are supported by NCSP, need to access, process and write data in the ENDF and/or GNDS format. Since the codes need to be kept

current with the ENDF format and content, it is important that RNSD personnel is involved in the governance of the format as well as in the development of the API to ensure that our data needs are adequately

addressed. In addition, influencing the physics checks that are applied to the data in any new ENDF library will ensure that the final library (after

processing) can be used as is, as physics checks relevant to our transport codes

are applied before the release of any updated ENDF library.

SITES OECD Conference Center, 2, rue André Pascal – 75016 Paris

**VISITED:** 

### **ABSTRACT:**

Attended EG-GNDS, SG-43 meeting to discuss the new GNDS format for the ENDF data. Presented the status of GNDS processing in AMPX and reported errors in the current ENDF->GNDS translation back to group. It was discussed when the official release of the GNDS format will occur. The decision was to test the current version as a beta version and only allow minor changes to the format until the final planned release of GNDS 2.0, planned at the next WPEC meeting. In addition we discussed whether we can develop an API for the format that allows other users to more easily adopt the new format in their codes.

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### REPORT OF FOREIGN TRAVEL

### Dorothea Wiarda OECD Headquarters, Paris, France 14-18 May 2018

### **PURPOSE OF TRAVEL**

Participate in the sub-group meetings for the OECD/NEA Working Party Evaluation Cooperation (WPEC), specifically: SG-43, EG-GNDS, SG-44, and SG-45. EG-GNDS was established for the long-time governance of the ENDF/GNDS format. The SG-43 was established to provide and API and physics checks for the new ENDF format. The data processing code AMPX, used to generate cross section libraries for SCALE and the analysis code SAMMY, both of which are supported by NCSP, need to access, process and write data in the ENDF and/or GNDS format. Since the codes need to be kept current with the ENDF format and content, it is important that RNSD personnel is involved in the governance of the format as well as in the development of the API to ensure that our data needs are adequately addressed. In addition, influencing the physics checks that are applied to the data in any new ENDF library will ensure that the final library (after processing) can be used as is, as physics checks relevant to our transport codes are applied before the release of any updated ENDF library.

### **Itinerary**

05/12/18 – 05/13/18 Travel from Knoxville, USA to Paris France

05/14/18 – 05/16/18 30th WPEC Meetings (workshop agenda attached)

05/17/18 Travel from Paris, France to Knoxville, USA

30th WPEC Meetings (day-by-day agenda)

05/14/18

Attended SG-45 (VANDAL) meeting. It was discussed whether the different laboratories could contribute parts of their validation suites to a common database of input decks and results. It was decided that the NEA can probably provide a GIT repository for this purpose, while allowing the different laboratories ownership of the data but also allow sharing and checking. It was further discussed how the different laboratories do QA on their validation suite (usually one person edits the input, followed by a check by a different person). Should the benchmarks considered only collect k-eff values or also other data. It was decided that pulsed sphere experiments with neutron and gamma spectra would also initially be of interest. In addition, it was discussed whether the benchmarks are good enough to tune data libraries and how to communicate that information to the evaluators. Talks included a presentation of how AMPX was used to process ROSFOND data and validate the library, a short overview of pulse sphere benchmark and a comparison of benchmark results from IRSN, Los Alamos and ORNL.

Action items include:

A small group of participants will suggest a common naming convention for the benchmarks in the database.

A small group will try to develop a suitable format to communicate the results of the benchmarks from different codes.

A small group will investigate what other benchmarks and outputs beside critical experiments are of interest to the larger group.

05/15/18

Attended the SG-42 (TSL data) and the joint SG-42, SG-44, GNDS session. In the morning session it was discussed what new formats in GNDS are needed to store the new information available for TSL evaluations. The current version of LEAPR available with NJOY is not compatible with the new evaluations, but the new program FFLASH is not yet available for wider distribution. While the final results are normally given in S(alpha,beta) form, it would be nice to add the LEARP input to the GNDS file format. Holmes compared calculations using their new scattering kernel for water with neutron die-away experiments to ensure that the data are sensitive enough to show differences in the evaluations. In the afternoon session it was discussed what the formats for the covariances matrices for the thermal moderator data need to be and how to add them to GNDS. Retroactive creation of covariance data in the thermal range was discussed and how the data can be grouped to avoid too large a covariance matrix. In addition it was discussed whether files with random S(alpha,beta) was better than to give a covariance matrix, to capture the non-linearity in the model. If the LEAPR input is given in the ENDF file, it was discussed whether the covariance for the phonon spectrum can be given.

05/16/18

Attended the SG-GNDS meeting in the morning. This included giving a status report on the current status of GNDS processing in AMPX. The current status of GNDS itself was discussed and when we will declare a stable GNDS 2.0 format. Currently the format is tested by a round-trip in LLNL's code FUDGE between ENDF->GNDS->ENDF and by using the GNDS formatted files in LNL transport codes. It was discussed how to streamline the documentation of the GNDS format so that it is in sync with the current implementation. In the afternoon, attended the SG-43 session and gave a more detailed report on how AMPX reads the GNDS data, see attached presentation. LLNL presented the API they are currently using to access GNDS formatted files in their transport codes. Different thoughts on a suitable API were discussed, which mainly concentrated on the lower level of the access to the file. In the second part of the afternoon, we discussed which physics test can be applied to a GNDS formatted file to ensure that the data are consistent. It is important that certain tests, like whether the cross section is positive, can only be done after processing. Action items for ORNL include to add ideas for physics test for resonance data into the WIKI and to outline the higher-level API currently used for AMPX on the WIKI in more detail.

### **DISTRIBUTION**

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